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RANDOM WALK AND THE THEORY OF BROWNIAN MOTION*

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1. Introduction. In 1827 an English botanist, Robert Brown, noticed that small particles suspended in fluids perform peculiarly erratic movements. This phenomenon, which can also be observed in gases, is referred to as Brownian motion. Although it soon became clear that Brownian motion is an outward manifestation of the molecular motion postulated by the kinetic theory of matter, it was not until 1905 that Albert Einstein first advanced a satisfactory theory.

The theory was then considerably generalized and extended by the Polish physicist Marjan Smoluchowski, and further important contributions were made by Fokker, Planck, Burger, Fürth, Ornstein, Uhlenbeck, Chandrasekhar, Kramers and others [1]. On the purely mathematical side various aspects of the theory were analyzed by Wiener, Kolomgoroff, Feller, Lévy, Doob, and Fortet [2]. Einstein considered the case of the *free* particle, that is, a particle on which no forces other than those due to the molecules of the surrounding medium are acting. His results can be briefly summarized as follows.

Consider the motion of the projection of the free particle‡ on a straight line which we shall call the x -axis. What one wants is the probability

$$\int_{x_1}^{x_2} P(x_0 | x; t) dx$$

that at time t the particle will be between x_1 and x_2 if it was at x_0 at time $t=0$. Einstein was then able to show that the "probability density" $P(x_0 | x; t)$ § must satisfy the partial differential equation

$$(1) \quad \frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2},$$

where D is a certain physical constant. The conditions imposed on P are

$$\begin{aligned} (a) \quad & P \geq 0 \\ (2) \quad (b) \quad & \int_{-\infty}^{\infty} P(x_0 | x; t) dx = 1 \\ (c) \quad & \lim_{t \rightarrow 0} P(x_0 | x; t) = 0, \quad \text{for } x \neq x_0. \end{aligned}$$

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‡ In what follows we shall identify this projection with the particle itself and hence consider the so-called one-dimensional Brownian motion.

§ The notation $P(x_0 | x; t)$ and $P(n | m; s)$ for conditional probabilities is that used by Wang and Uhlenbeck [1]. It does not conform with the notation adopted in the statistical literature. Had we adopted the latter notation we would write $P(x; t | x_0)$ and $P(m; s | n)$.

Conditions (a) and (b) are the usual ones imposed upon a probability density and condition (c) expresses the *certainty* that at $t=0$ the particle was at x_0 . It is well known that (1) and (2) imply that

$$(3) \quad P(x_0 | x; t) = \frac{1}{2\sqrt{\pi Dt}} e^{-(x-x_0)^2/4Dt}$$

and that the solution (3) is unique.

The greatness of Einstein's contribution was not, however, solely due to the derivation of (1), and hence (3). From the point of view of physical applications it was equally, or perhaps even more, important that he was able to show that

$$(4) \quad D = \frac{2RT}{Nf},$$

where R is the universal gas constant, T the absolute temperature, N the Avogadro number, and f the friction coefficient. The friction coefficient f , in the case the medium is a liquid or a gas at ordinary pressure, can in turn be expressed in terms of viscosity and the size of the particle [3].

It was relation (4) that made possible the determination of the Avogadro number from Brownian motion experiments, an achievement for which Perrin was awarded the Nobel prize in 1926. However, the derivation of (4) belongs to physics proper, and presents no particular mathematical interest; we shall therefore not be concerned with it in the sequel.

As soon as the theory for the free particle was established, a natural question arose as to how it should be modified in order to take into account outside forces as, for example, gravity. Assuming that the outside force acts in the direction of the x -axis and is given by an expression $F(x)$, Smoluchowski has shown that (1) should in this case be replaced by

$$(5) \quad \frac{\partial P}{\partial t} = -\frac{1}{f} \frac{\partial}{\partial x} (PF) + D \frac{\partial^2 P}{\partial x^2}.$$

Two cases of special interest and importance are:

$F(x) = -a$; field of constant force (for example, gravity).

$F(x) = -bx$; elastically bound particle (for example, small pendulum).

At this point it must be strongly emphasized that theories based on (1) and (5) are only approximate. They are valid only for relatively large t and, in the case of an elastically bound particle, only in the overdamped case, that is, when the friction coefficient is sufficiently large. These limitations of the theory were already recognized by Einstein and Smoluchowski but are often disregarded by writers who stress that in Brownian motion the velocity of the particle is infinite. This paradoxical conclusion is a result of stretching the theory beyond the bounds of its applicability. An improved theory (known as "exact") was advanced by Uhlenbeck and Ornstein and by Kramers. The Uhlenbeck-Orn-

stein approach was further elaborated by Chandrasekhar and Doob.

In what follows we shall be concerned with a discrete approach to the Einstein-Smoluchowski (approximate) theory. This approach was first suggested by Smoluchowski himself; it consists in treating Brownian motion as a discrete random walk. Smoluchowski used this approach only in connection with a free particle but we shall also treat other classical cases. Moreover, a re-interpretation of one of the discrete models will allow us to discuss the important question of recurrence and irreversibility in thermodynamics.

The main advantages of a discrete approach are pedagogical, inasmuch as one is able to circumvent various conceptual difficulties inherent to the continuous approach. It is also not without a purely scientific interest and it is hoped that it may suggest various generalizations which will contribute to the development of the Calculus of Probability.

2. The free particle. Imagine a particle which moves along the x -axis in such a way that in each step it can move either Δ to the right or Δ to the left, the duration of each step being τ . The fact that we are dealing with a free particle is interpreted by assuming that the probabilities of moving to the right or to the left are equal, and hence each equal $\frac{1}{2}$. Instead of $P(x_0|x; t)$ we now consider $P(n\Delta|m\Delta; s\tau) = P(n|m; s)$ which is the probability that the particle is at $m\Delta$ at time $s\tau$, if at the beginning it was at $n\Delta$. Noticing that $P(n|m; s)$ is also the probability that after s games of "heads or tails" the gain of a player is $\nu = m - n$, we can write

$$(6) \quad P(n|m; s) = \begin{cases} \frac{1}{2^s} \frac{s!}{\left(\frac{s+|\nu|}{2}\right)! \left(\frac{s-|\nu|}{2}\right)!} & \text{if } |\nu| \leq s \text{ and } |\nu| + s \text{ is even,} \\ 0 & \text{otherwise.} \end{cases}$$

Suppose now that Δ and τ approach 0 in such a way that

$$(7) \quad \frac{\Delta^2}{2\tau} = D, \quad n\Delta \rightarrow x_0, \quad s\tau = t.$$

It then follows from the classical Laplace-De Moivre theorem [4] that

$$(8) \quad \lim_{x_1 < m\Delta < x_2} \sum_{x_1 < m\Delta < x_2} P(n|m; s) = \frac{1}{2\sqrt{\pi Dt}} \int_{x_1}^{x_2} e^{-(x-x_0)^2/4Dt} dx,$$

and hence the fundamental result of Einstein emerges as a consequence of what in probability theory we call a "limit theorem."

It is both important and instructive to point out a striking formal connection between the discrete (random walk) and the continuous (Einstein) approaches. We notice that $P(n|m; s)$ satisfies the difference equation

$$(9) \quad P(n|m; s+1) = \frac{1}{2}P(n|m-1; s) + \frac{1}{2}P(n|m+1; s),$$

which we write in the equivalent form

$$(10) \quad \frac{P(n\Delta | m\Delta; (s+1)\tau) - P(n\Delta | m\Delta; s\tau)}{\tau} = \frac{\Delta^2}{2\tau} \left\{ \frac{P(n\Delta | (m+1)\Delta; s\tau) - 2P(n\Delta | m\Delta; s\tau) + P(n\Delta | (m-1)\Delta; s\tau)}{\Delta^2} \right\}.$$

In the limit (7) this difference equation goes over formally into the differential equation

$$(11) \quad \frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2},$$

which as noted before was the basis of Einstein's theory. This formal connection between the two approaches can be made rigorous, but we shall not go into this. However, we shall use it as a guiding heuristic principle in constructing models of Brownian motion when outside forces are taken into account.

Finally, let us mention that it is the relation

$$\frac{\Delta^2}{2\tau} = D,$$

which is responsible for the conclusion that the velocity of a Brownian particle is infinite. In fact, in our model, the ratio Δ/τ plays the role of the instantaneous velocity and it obviously approaches infinity as $\Delta \rightarrow 0$.

3. Particle in a field of constant force and in the presence of a reflecting barrier. We again consider random walk along the x -axis in which a particle can move Δ to the right or Δ to the left, the duration of each step being τ . We now introduce the following new assumptions:

(a) The probability of a move to the right is $q = \frac{1}{2} - \beta\Delta$, and consequently the probability of a move to the left is $p = \frac{1}{2} + \beta\Delta$. Here β is a certain physical constant, and Δ must be chosen sufficiently small so that $q > 0$.

(b) When the particle reaches the point $x=0$ (*reflecting barrier*) it must, in the next step, move Δ to the right.

Without the assumption (b) the problem would be quite simple and of no great physical interest. In actual experiments with heavy Brownian particles, like those of Perrin, the bottom of the container acts as a reflecting barrier and the elucidation of its influence on the Brownian motion is of considerable theoretical interest.

This problem has been solved by Smoluchowski, on the basis of his equation (5) but we shall show that one can solve the discrete problem and obtain Smoluchowski's result by passing to a limit.

Assuming that the particle starts from $n\Delta \geq 0$ (n an integer) we seek an explicit expression for $P(n|m; s)$. We first notice that $P(n|m; s)$ satisfies, for

$m \geq 2$, the difference equation

$$(12) \quad P(n | m; s+1) = qP(n | m-1; s) + pP(n | m+1; s),$$

and that for $m=1$ and $m=0$ we have

$$(12a) \quad P(n | 1; s+1) = P(n | 0; s) + pP(n | 2; s),$$

$$(12b) \quad P(n | 0; s+1) = pP(n | 1; s).$$

We also have the initial condition

$$(13) \quad P(n | m; 0) = \delta(m, n),$$

where $\delta(m, n)$ denotes, as usual, the Kronecker delta.

The difference equation (12) when rewritten in the form analogous to (10) can be shown to go over formally (in the limit $\Delta \rightarrow 0$, $\tau \rightarrow 0$, $\Delta^2/2\tau = D$, $n\Delta \rightarrow x_0$, $m\Delta \rightarrow x$, $s\tau = t$) into the differential equation

$$(14) \quad \frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2} + 4\beta D \frac{\partial P}{\partial x},$$

which is of the form (5) with $F(x) = -a = -4\beta Df$.

To find $P(n | m; s)$ we use a method which is basic in the study of the so-called Markoff chains, of which our problem is but a particular example, and which in its essentials goes back to Poincaré [5]. Let $(p)_s$ be the (infinite) vector

$$(15) \quad (p)_s = \begin{bmatrix} P(n | 0; s) \\ P(n | 1; s) \\ P(n | 2; s) \\ \vdots \\ \vdots \end{bmatrix}$$

and A the infinite matrix

$$(16) \quad A = \begin{pmatrix} 0 & p & 0 & 0 & 0 & \dots \\ 1 & 0 & p & 0 & 0 & \dots \\ 0 & q & 0 & p & 0 & \dots \\ 0 & 0 & q & 0 & p & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}.$$

Then, the difference equation (12), (12a) and (12b), can be written in the matrix form as

$$(17) \quad (p)_{s+1} = A(p)_s.$$

Thus it follows immediately that

$$(18) \quad (p)_s = A^s(p)_0,$$

where $(p)_0$ is the vector

$$(p)_0 = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ \vdots \end{pmatrix},$$

1 being the n th component, the components being numbered from zero on. Interpreting (18), we see that

$$(19) \quad P(n | m; s) = \text{the } (m, n) \text{ element of } A^s.$$

To make use of (19), we notice that if $R > n + s$ and we consider the finite matrix A_R , which is the upper left R by R submatrix of A , then for $m < R$

$$(20) \quad \text{the } (m, n) \text{ element of } A^s = \text{the } (m, n) \text{ element of } A_R^s,$$

or equivalently,

$$(21) \quad \text{the } (m, n) \text{ element of } A^s = \lim_{R \rightarrow \infty} \text{the } (m, n) \text{ element of } A_R^s.$$

For each R there exist matrices P_R and Q_R such that

$$(22) \quad P_R Q_R = I$$

and

$$(23) \quad A_R = P_R \begin{bmatrix} \lambda_0(R) & & & 0 \\ & \lambda_1(R) & & \\ & & \ddots & \\ 0 & & & \lambda_{R-1}(R) \end{bmatrix} Q_R,$$

$\lambda_0(R), \lambda_1(R), \dots, \lambda_{R-1}(R)$ being the eigenvalues of the matrix A_R . To simplify the notation we write λ_j for $\lambda_j(R)$.

Multiplying the matrix A_R s times by itself and making use of (22), we obtain

$$(24) \quad A_R^s = P_R \begin{bmatrix} \lambda_0^s & & & 0 \\ & \lambda_1^s & & \\ & & \ddots & \\ 0 & & & \lambda_{R-1}^s \end{bmatrix} Q_R$$

and one can calculate the (m, n) element of A_R^s explicitly provided the diag-

onalization (23) can be performed explicitly. This indeed is the case.

Let $(x)_0, (x)_1, \dots, (x)_{R-1}$ be the "right" and $(y)_0, (y)_1, \dots, (y)_{R-1}$ the "left" eigenvectors belonging respectively to the eigenvalues $\lambda_0, \lambda_1, \dots, \lambda_{R-1}$. In other words, for $k=0, 1, \dots, R-1$, we have

$$\begin{aligned} A_R(x)_k &= \lambda_k(x)_k, \\ A_R'(y)_k &= \lambda_k(y)_k, \end{aligned}$$

where A_R' is the transpose of A_R .

Suppose furthermore that the vectors can be so normalized that

$$(25) \quad (x)_k \cdot (y)_k = 1, \quad k = 0, 1, \dots, R-1,$$

where $(x)_k \cdot (y)_k$ is the inner (dot) product of the vectors. Since it is well known that

$$(x)_j \cdot (y)_k = 0 \quad \text{for } \lambda_j \neq \lambda_k$$

we see that, in the case when all the eigenvalues are distinct, we can take as P_R the matrix whose columns are the vectors $(x)_k$ and for Q_R the matrix whose rows are the vectors $(y)_k$.

In order to determine the eigenvalues and the right eigenvectors we consider the system of linear equations

$$\begin{aligned} (26) \quad & p x_1 = \lambda x_0 \\ & x_0 + p x_2 = \lambda x_1 \\ & q x_1 + p x_3 = \lambda x_2 \\ & \dots \dots \dots \\ & q x_{R-2} = \lambda x_{R-1}, \end{aligned}$$

and the extended infinite system

$$\begin{aligned} (27) \quad & p x_1 = \lambda x_0 \\ & x_0 + p x_2 = \lambda x_1 \\ & \dots \dots \dots \\ & q x_{R-1} + p x_{R+1} = \lambda x_R \\ & \dots \dots \dots \end{aligned}$$

If we can find non-trivial solutions of (27), for which

$$(28) \quad x_R = 0,$$

we will have found solutions of (26).

It turns out that (28) will yield an equation in λ which has R distinct roots and thus our procedure gives us all eigenvalues, and consequently all right eigenvectors. Multiplying the members of the equations of (27) by 1,

z, z^2, \dots , and adding, we obtain formally

$$x_0 z + q \sum_1^{\infty} x_k z^{k+1} + p \sum_1^{\infty} x_k z^{k-1} = \lambda \sum_0^{\infty} x_k z^k$$

or, upon introducing the abbreviation,

$$(29) \quad f(z) = \sum_0^{\infty} x_k z^k,$$

we have

$$(30) \quad x_0 z + qz[f(z) - x_0] + \frac{p}{z} [f(z) - x_0] = \lambda f(z).$$

From (30) we obtain

$$(31) \quad f(z) = \frac{p}{q} x_0 \left\{ -1 + \frac{1 - \lambda z}{qz^2 - \lambda z + p} \right\},$$

and since this function is analytic in the neighborhood of zero the formal procedure used above can be justified.

Let ρ_1 and ρ_2 be the *reciprocals* of the roots of

$$(32) \quad qz^2 - \lambda z + p = 0.$$

We have then

$$(33) \quad f(z) = \frac{p}{q} x_0 \left\{ -1 + \frac{1 - \lambda z}{p(1 - \rho_1 z)(1 - \rho_2 z)} \right\},$$

and introducing partial fractions,

$$(34) \quad \frac{1 - \lambda z}{p(1 - \rho_1 z)(1 - \rho_2 z)} = \frac{1}{p} \frac{\lambda - \rho_1}{\rho_2 - \rho_1} \frac{1}{1 - \rho_1 z} + \frac{1}{p} \frac{\rho_2 - \lambda}{\rho_2 - \rho_1} \frac{1}{1 - \rho_2 z}.$$

Thus

$$(35) \quad x_k = \frac{x_0}{q} \left(\frac{\lambda - \rho_1}{\rho_2 - \rho_1} \rho_1^k + \frac{\rho_2 - \lambda}{\rho_2 - \rho_1} \rho_2^k \right) \quad \text{for } k \geq 1,$$

and, in particular, the equation $x_R = 0$ assumes the form

$$(36) \quad \frac{\lambda - \rho_1}{\rho_2 - \rho_1} \rho_1^R + \frac{\rho_2 - \lambda}{\rho_2 - \rho_1} \rho_2^R = 0.$$

Equation (36) must now be solved for λ . Assuming R to be even, and seeking solutions in the form

$$\lambda = 2\sqrt{pq} \cos \Theta, \quad 0 \leq \Theta \leq \pi,$$

we are led to the equation

$$\frac{\tan R\Theta}{\tan \Theta} = \frac{1}{2p-1}.$$

For $R > (2p-1)^{-1}$ this equation is seen to have $R-2$ distinct roots, $\Theta_1, \Theta_2, \dots, \Theta_{R-2}$, which lie in the subintervals

$$\left(\frac{j\pi}{R} - \frac{\pi}{2R}, \frac{j\pi}{R} + \frac{\pi}{2R} \right),$$

where j ranges through the integers from 1 to $R-1$ with the exception of $j=R/2$. Corresponding to $\Theta_1, \Theta_2, \dots, \Theta_{R-2}$ we have $R-2$ distinct eigenvalues,

$$\lambda_k = 2\sqrt{pq} \cos \Theta_k, \quad k = 1, 2, \dots, R-2,$$

and the components of the right eigenvector belonging to λ_k can be written in the form

$$x_k^{(m)} = a_k \left(\frac{q}{p} \right)_*^{m/2} \left(\cos m\Theta_k - 2\beta\Delta \frac{\sin m\Theta_k}{\sin \Theta_k} \right),$$

where

$$\left(\frac{q}{p} \right)_*^\mu = \begin{cases} \left(\frac{q}{p} \right)^\mu & \text{if } \mu > 0, \\ q & \text{if } \mu = 0, \end{cases}$$

and a_k is a normalizing constant which will be fixed later. For sufficiently large R the remaining eigenvalues λ_0 and λ_{R-1} can be shown to be given by the formulas

$$\lambda_0 = 2\sqrt{pq} \cosh \theta_0, \quad \lambda_{R-1} = -\lambda_0,$$

where θ_0 is the only positive root of the equation

$$\frac{\tanh R\theta}{\tanh \theta} = \frac{1}{2p-1}.$$

The components of the corresponding right eigenvectors are given by the expressions

$$\begin{aligned} x_0^{(m)} &= a_0 \left(\frac{q}{p} \right)_*^{m/2} \left(\cosh m\theta_0 - 2\beta\Delta \frac{\sinh m\theta_0}{\sinh \theta_0} \right) \\ x_{R-1}^{(m)} &= a_{R-1} (-1)^m \left(\frac{q}{p} \right)_*^{m/2} \left(\cosh m\theta_0 - 2\beta\Delta \frac{\sinh m\theta_0}{\sinh \theta_0} \right). \end{aligned}$$

It remains now to find the left eigenvectors. This can be accomplished in exactly the same manner and we merely quote the results. We obtain

$$y_k^{(m)} = b_k \left(\frac{p}{q} \right)^{m/2} \left(\cos m\Theta_k - 2\beta\Delta \frac{\sin m\Theta_k}{\sin \Theta_k} \right)$$

for $m=0, 1, \dots, R-1$; $k=1, 2, \dots, R-2$, and

$$y_0^{(m)} = b_0 \left(\frac{p}{q} \right)^{m/2} \left(\cosh m\theta_0 - 2\beta\Delta \frac{\sinh m\theta_0}{\sinh \theta_0} \right)$$

$$y_{R-1}^{(m)} = b_{R-1} (-1)^m \left(\frac{p}{q} \right)^{m/2} \left(\cosh m\theta_0 - 2\beta\Delta \frac{\sinh m\theta_0}{\sinh \theta_0} \right).$$

To satisfy the normalization conditions (25) we must have

$$(37) \quad a_k b_k \left(q + \sum_{m=1}^{R-1} f_m^2(\Theta_k) \right) = 1, \quad k = 1, 2, \dots, R-2,$$

$$(38) \quad a_k b_k \left(q + \sum_{m=1}^{R-1} F_m^2(\theta_0) \right) = 1, \quad k = 0, R-1,$$

where

$$f_m(\Theta) = \cos m\Theta - 2\beta\Delta \frac{\sin m\Theta}{\sin \Theta}$$

and

$$F_m(\theta) = \cosh m\theta - 2\beta\Delta \frac{\sinh m\theta}{\sinh \theta}.$$

We can, of course, put $a_0 = a_1 = \dots = a_{R-1} = 1$, and determine the b 's from (37) and (38). Referring back to (19), (20), and (24), and recalling that columns of P_R are the right eigenvectors $(x)_k$, and the rows of Q_R are the left eigenvectors $(y)_k$, we obtain

$$(39) \quad P(n | m; s) = \sum_{k=0}^{R-1} \lambda_k^s x_k^{(m)} y_k^{(n)},$$

or, more explicitly,

$$(40) \quad P(n | m; s) = b_0 (2\sqrt{pq} \cosh \theta_0)^s \left(\frac{p}{q} \right)^{n/2} \left(\frac{q}{p} \right)_*^{m/2} F_m(\theta_0) F_n(\theta_0) [1 + (-1)^{m+n+s}]$$

$$+ \left(\frac{p}{q} \right)^{n/2} \left(\frac{q}{p} \right)_*^{m/2} (2\sqrt{pq})^s \sum_{k=1}^{R-2} b_k \cos^s \Theta_k f_m(\Theta_k) f_n(\Theta_k).$$

Making use of (21), we can achieve considerable simplification by letting $R \rightarrow \infty$. In fact, it can be shown that

$$(41) \quad P(n | m; s) = \frac{p-q}{2pq} \left(\frac{q}{p} \right)_*^m [1 + (-1)^{m+n+s}]$$

$$+ \frac{2}{\pi} \left(\frac{p}{q} \right)^{n/2} \left(\frac{q}{p} \right)^{m/2} (2\sqrt{pq})^s \int_0^\pi \cos^s \Theta \frac{\tan^2 \Theta}{(p-q)^2 + \tan^2 \Theta} f_n(\Theta) f_m(\Theta) d\Theta.$$

Although in various places we have tacitly assumed that p and q are different from $\frac{1}{2}$, the final formula (41) can easily be seen to be valid also for the case $p=q=\frac{1}{2}$. In this case (free particle in the presence of a reflecting barrier) the formula assumes the remarkably simple form

$$(42) \quad P(n | m; s) = \frac{2}{\pi} (1)_*^{m/2} \int_0^\pi \cos^s \Theta \cos m\Theta \cos n\Theta d\Theta,$$

and the right member can be expressed in terms of binomial coefficients. This formula can also be derived in a much simpler way using, for instance, the classical method of images.

In the limit

$$\Delta \rightarrow 0, \quad \tau \rightarrow 0, \quad \frac{\Delta^2}{2\tau} = D, \quad n\Delta \rightarrow x_0, \quad s\tau = t,$$

one can show that

$$\lim_{x_1 < m\Delta < x_2} \sum P(n | m; s) = \int_{x_1}^{x_2} P(x_0 | x; t) dx,$$

where

$$(43) \quad P(x_0 | x; t) = 4\beta e^{-4\beta x} + e^{-2\beta(x-x_0)} e^{-4\beta^2 D t} \frac{2}{\pi} \int_0^\infty e^{-D y^2 t} \frac{y^2}{4\beta^2 + y^2} g(x, y) g(x_0, y) dy,$$

and

$$g(x, y) = \cos xy - 2\beta(\sin xy)/y.$$

The proof of this theorem is not elementary inasmuch as it utilizes the so called "continuity theorem for Fourier-Stieltjes transforms" [6]. Formula (43) can be shown to be equivalent with Smoluchowski's formula given in [1].

4. An elastically bound particle. Again the particle can move either Δ to the right or Δ to the left, and the duration of each step is τ . However, the probability of moving in either direction depends on the position of the particle. More precisely, if the particle is at $k\Delta$ the probabilities of moving right or left are

$$\frac{1}{2} \left(1 - \frac{k}{R} \right) \quad \text{or} \quad \frac{1}{2} \left(1 + \frac{k}{R} \right),$$

respectively. R is a certain integer, and possible positions of the particle are limited by the condition $-R \leq k \leq R$. The basic probabilities $P(n | m; s)$ now satisfy the difference equation

$$(44) \quad P(n|m; s+1) = \frac{R+m+1}{2R} P(n|m+1; s) + \frac{R-m+1}{2R} P(n|m-1; s),$$

which must be solved with the initial condition

$$(45) \quad P(n|m; 0) = \delta(m, n).$$

In the limit

$$\begin{aligned} \Delta \rightarrow 0, \quad \tau \rightarrow 0, \quad R \rightarrow \infty, \quad \frac{\Delta^2}{2\tau} = D, \quad \frac{1}{R\tau} \rightarrow \gamma, \\ s\tau = t, \quad n\Delta \rightarrow x_0, \quad m\Delta \rightarrow x, \end{aligned}$$

the difference equation (44) is seen to go over formally into the differential equation

$$(46) \quad \frac{\partial P}{\partial t} = \gamma \frac{\partial(xP)}{\partial x} + D \frac{\partial^2 P}{\partial x^2}$$

which is Smoluchowski's equation (5) with $F(x) = -x/\gamma f$.

The discrete problem in a different form and in a different connection was first proposed and discussed by P. and T. Ehrenfest in 1907 [7]. In the next section we shall discuss their original formulation. A fairly detailed treatment was given by Schrödinger and Kohlrausch in 1926 [8] and a brief exposition can be found in the review article of Wang and Uhlenbeck [1]. It seems that Schrödinger and Kohlrausch were the first to point out the connection between the Ehrenfest model and Brownian motion of an elastically bound particle. However, an explicit solution of (44) with the initial condition (45) was apparently not known. I have recently found such a solution using the matrix method described in Section 3 [9]. Instead of the infinite matrix of that section we must now consider the finite matrix

$$(47) \quad B = \begin{pmatrix} 0 & \frac{1}{2R} & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & \frac{2}{2R} & 0 & 0 & \dots & 0 \\ 0 & 1 - \frac{1}{2R} & 0 & \frac{3}{2R} & 0 & \dots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \dots & \dots & \frac{1}{2R} & 0 \end{pmatrix}$$

and the problem is again reduced to finding the eigenvalues $\lambda_{-R}, \lambda_{-R+1}, \dots, \lambda_0, \dots, \lambda_{R-1}, \lambda_R$ of B and matrices P and Q such that

$$\begin{aligned} \frac{1}{2R} x_{2R-1} + \frac{2R+1}{2R} x_{2R+1} &= \lambda x_{2R} \\ \frac{2R+2}{2R} x_{2R+2} &= \lambda x_{2R+1} \\ &\dots \end{aligned}$$

If we can find non-trivial solutions of (52) for which

$$(53) \quad x_{2R+1} = 0$$

we will have found solutions of (51). It will turn out that this procedure will again yield all eigenvalues and right eigenvectors. Multiplying the members of the equations of (52) by $1, z, z^2, \dots$, and adding, we obtain formally

$$\sum_{k=0}^{\infty} \left(1 - \frac{k}{2R}\right) x_k z^{k+1} + \sum_{k=0}^{\infty} \frac{k}{2R} x_k z^{k-1} = \lambda \sum_{k=0}^{\infty} x_k z^k,$$

or, introducing the abbreviation

$$f(z) = \sum_{k=0}^{\infty} x_k z^k,$$

$$zf(z) - \frac{z^2}{2R} f'(z) + \frac{1}{2R} f'(z) = \lambda f(z).$$

We thus get the differential equation

$$(54) \quad f'(z) = 2R \frac{\lambda - z}{1 - z^2} f(z),$$

whose solution satisfying $f(0) = x_0$ is easily found to be

$$(55) \quad f(z) = x_0 (1 - z)^{R(1-\lambda)} (1 + z)^{R(1+\lambda)}.$$

Since $f(z)$ is analytic in the neighborhood of $z=0$ the formal procedure can be justified.

We now notice that if

$$(56) \quad \lambda = \frac{j}{R}, \quad j = -R, -R+1, \dots, 0, \dots, R-1, R,$$

$f(z)$ is a polynomial of degree $2R$, and hence $x_{2R+1}=0$. The numbers (56) are thus seen to be eigenvalues of B and, since there are $2R+1$ of them, we see that we have found *all* the eigenvalues. It also follows that the components of the right eigenvector belonging to the eigenvalue $\lambda_j=j/R$ can be taken as

$$C_0^{(j)} = 1, C_1^{(j)}, C_2^{(j)}, \dots, C_{2R}^{(j)},$$

where the C 's are defined by the identity

$$(57) \quad (1-z)^{R-j}(1+z)^{R+j} \equiv \sum_{k=0}^{2R} C_k^{(j)} z^k.$$

So far we have followed very closely the procedure described in Section 3. Surprisingly enough, we encounter unexpected difficulties in trying to carry out the analogy still further and determine by similar means the left eigenvectors.

To find the matrix Q we resort to a different method. Let us first recall that P can be taken as the matrix whose j th column (for convenience columns and rows are numbered from $-R$ to R) is

$$\begin{pmatrix} 1 \\ C_1^{(j)} \\ C_2^{(j)} \\ \vdots \\ C_{2R}^{(j)} \end{pmatrix}.$$

Matrix Q must satisfy the equation

$$P'Q' = I,$$

which is an immediate consequence of the equation $PQ = I$, and hence denoting by $\alpha_{-R}, \dots, \alpha_0, \dots, \alpha_R$, the consecutive elements of the j th column of Q' , we must have

$$(58) \quad \sum_{k=-R}^R C_{R+r}^{(k)} \alpha_k = \delta(j, r), \quad r = -R, \dots, R.$$

From (58) it follows that

$$\begin{aligned} z^{R+j} &= \sum_{r=-R}^R \delta(j, r) z^{R+r} = \sum_{r=-R}^R z^{R+r} \sum_{k=-R}^R C_{R+r}^{(k)} \alpha_k = \sum_{k=-R}^R \alpha_k \sum_{r=-R}^R C_{R+r}^{(k)} z^{R+r} \\ &= \sum_{k=-R}^R \alpha_k \sum_{s=0}^{2R} C_s^{(k)} z^s, \end{aligned}$$

or, by virtue of (57),

$$z^{R+j} = \sum_{k=-R}^R \alpha_k (1-z)^{R-k} (1+z)^{R+k} = (1-z)^{2R} \sum_{l=0}^{2R} \alpha_{l-R} \left(\frac{1+z}{1-z} \right)^l.$$

Thus

$$(59) \quad \frac{z^{R+j}}{(1-z)^{2R}} = \sum_{l=0}^{2R} \alpha_{l-R} \left(\frac{1+z}{1-z} \right)^l.$$

Let

$$\zeta = \frac{1+z}{1-z},$$

so that

$$z = -\frac{1-\zeta}{1+\zeta} \quad \text{and} \quad 1-z = \frac{2}{1+\zeta}.$$

In terms of ζ (59) assumes the form

$$(60) \quad \frac{(-1)^{R+j}}{2^{2R}} (1-\zeta)^{R+j} (1+\zeta)^{R-j} = \sum_{l=0}^{2R} \alpha_{l-R} \zeta^l,$$

and since by (57)

$$(1-\zeta)^{R+j} (1+\zeta)^{R-j} = \sum_{l=0}^{2R} C_l^{(-j)} \zeta^l,$$

we obtain, by comparing coefficients of corresponding powers of ζ ,

$$\alpha_{l-R} = \frac{(-1)^{R+j}}{2^{2R}} C_l^{(-j)},$$

or finally,

$$(61) \quad \alpha_s = \frac{(-1)^{R+j}}{2^{2R}} C_{R+s}^{(-j)}.$$

Formula (61) determines explicitly the elements of Q' (and hence of Q), and it is now possible to write an explicit expression for $P(n|m; s)$. In fact, making use of (50), we obtain

$$(62) \quad P(n|m; s) = \frac{(-1)^{R+n}}{2^{2R}} \sum_{j=-R}^R \left(\frac{j}{R}\right)^s C_{R+j}^{(-n)} C_{R+m}^{(j)}.$$

In the limit

$$\Delta \rightarrow 0, \quad \tau \rightarrow 0, \quad \frac{\Delta^2}{2\tau} = D, \quad \frac{1}{R\tau} \rightarrow \gamma, \quad s\tau = t, \quad n\Delta \rightarrow x_0,$$

we have

$$\lim_{x_1 < m\Delta < x_2} \sum P(n|m; s) = \int_{x_1}^{x_2} P(x_0|x; t) dx,$$

where

$$(63) \quad P(x_0|x; t) = \frac{\sqrt{\gamma}}{\sqrt{2\pi D(1-e^{-2\gamma t})}} e^{-\gamma(x-x_0 e^{-\gamma t})^2 / 2\gamma(1-e^{-2\gamma t})}.$$

The proof is again made to depend on the continuity theorem for Fourier-Stieltjes transforms.

The frequency function (63) was first discovered by Lord Raleigh [10]. Its connection with Brownian motion of an elastically bound particle, in the strongly overdamped case, was established by Smoluchowski who arrived at it quite independently.

5. The Ehrenfest model. Irreversibility and recurrence. Imagine $2R$ balls numbered consecutively from 1 to $2R$, distributed in two boxes (I and II) so that at the beginning there are $R+n$, $-R \leq n \leq R$, balls in box I. We chose at random an integer between 1 and $2R$ (all these integers are assumed to be equiprobable) and move the ball, whose number has been drawn from the box in which it is, to the other box. This process is then repeated s times and we ask for the probability $Q(R+n | R+m; s)$ that after s drawings there should be $R+m$ balls in box I.

A moment's reflection will persuade one that this formulation (originally proposed by P. and T. Ehrenfest) [7] is equivalent to the random walk formulation of Section 4, if one interprets the excess over R of balls in box I as the displacement of the particle ($\Delta=1$). Thus

$$Q(R+n | R+m; s) = P(n | m; s),$$

where $P(n | m; s)$ has the meaning of Section 4.

In the present formulation we have a simple and convenient model of heat exchange between two isolated bodies of unequal temperatures. The temperatures are symbolized by the numbers of balls in the boxes and the heat exchange is not an orderly process, as in classical thermodynamics, but a random one like in the kinetic theory of matter. The realistic value of the model is greatly enhanced by the fact that the average excess over R of the number of balls in box I, namely, the quantity

$$\sum_{m=-R}^R m P(n | m; s)$$

can easily be shown to be equal to

$$(64) \quad n \left(1 - \frac{1}{R}\right)^s$$

which in the limit $R \rightarrow \infty$, $1/R\tau \rightarrow \gamma$, $s\tau = t$, gives

$$ne^{-\gamma t},$$

or the Newton law of cooling.

There are several proofs of (64) [11]. The most straightforward one, which is not however the simplest, is based on formula (62).

The Ehrenfest model is also particularly suited for the discussion of a famous paradox which at the turn of this century nearly wrecked Boltzmann's inspired

efforts to explain thermodynamics on the basis of kinetic theory. In classical thermodynamics the process of heat exchange of two isolated bodies of unequal temperatures is irreversible. On the other hand, if the bodies are treated as a dynamical system the famed "Wiederkehrrsatz" of Poincaré asserts that "almost every" state (except for a set of states which, when interpreted as points in phase space, form a set of Lebesgue measure 0) of the system will be, to an arbitrarily prescribed degree of accuracy, again approximately achieved. Thus, argued Zermelo, the irreversibility postulated in thermodynamics and the "recurrence" properties of dynamical systems are irreconcilable. Boltzmann then replied that the "Poincaré cycles" (time intervals after which states "nearly recur" for the first time,—the word "nearly" requiring further specification) are so long compared to time intervals involved in ordinary experiences that predictions based on classical thermodynamics can be fully trusted. This explanation, though correct in principle, was set forth in a manner which was not quite convincing and the controversy raged on. It was mainly through the efforts of Ehrenfest and Smoluchowski that the situation became completely clarified, and the irreversibility interpreted in a proper statistical manner.

It will now be easy to discuss this explanation by appealing to the Ehrenfest model. Let $P'(n|m; s)$ denote the probability that after s drawings (the duration of each drawing is τ), $R+m$ balls will be observed *for the first time* in box I if there were $R+n$ balls in that box at the beginning. In particular, $P'(n|n; s)$ is the probability that the recurrence time of the state " n " (defined by the presence of $R+n$ balls in box I) is $s\tau$. One can then show that

$$(65) \quad \sum_{s=1}^{\infty} P'(n|n; s) = 1,$$

or, in other words: *each state is bound to recur with probability 1*. This is the statistical analogue of the "Wiederkehrrsatz." One can show furthermore that the mean recurrence time, namely, the quantity

$$\theta_n = \sum_{s=1}^{\infty} s\tau P'(n|n; s)$$

is equal to

$$(66) \quad \tau \frac{(R+n)!(R-n)!}{(2R)!} 2^{2R}.$$

This is the statistical analogue of a "Poincaré cycle," and it tells us, roughly speaking, how long, on the average, one will have to wait for the state " n " to recur.

If $R+n$ and $R-n$ differ considerably, θ_n is enormous. For example, if $R=10000$, $n=10000$, $\tau=1$ second, we get

$$\theta = 2^{20000} \text{ seconds (of the order of } 10^{6000} \text{ years!).}$$

If on the other hand, $R+n$ and $R-n$ are nearly equal, θ_n is quite short. If in the above example we set $n=0$ we get (using Stirling's formula)

$$\theta \sim 100\sqrt{\pi} \text{ seconds} \sim 175 \text{ seconds.}$$

It was Smoluchowski who advanced the rule [12] that if one starts in a state with a long recurrence time the process will appear as irreversible. In our example if one starts with 20000 balls in one box and none in the other, one should observe, for a long time, an essentially irreversible flow of balls. On the other hand, if the mean recurrence time is short, there is no sense to speak about irreversibility.

We now give the proofs of (65) and (66). We shall base our considerations on a formula which Professor Uhlenbeck used for similar purposes in some of his unpublished notes. The formula in question is:

$$(67) \quad P(n | m; s) = P'(n | m; s) + \sum_{k=1}^{s-1} P'(n | m; k)P(m | m; s-k).$$

To convince oneself of the validity of this formula we divide all possible ways of reaching " m " from " n " in s steps into classes according to when " m " has been reached for the first time. We then observe that starting from " n " one can reach " m " in s steps in the following s mutually exclusive ways:

- (1) " m " is reached for the first time after s steps.
- (2) " m " is reached for the first time in 1 step and then, starting from " m " it is again reached in $s-1$ steps.
- (3) " m " is reached for the first time in 2 steps and then, starting from " m ", it is reached again in $s-2$ steps, and so forth. We note furthermore that the probability that " m " will be reached for the first time in k steps and then, starting from " m ," it will be reached again in $s-k$ steps, is

$$(68) \quad P'(n | m; k)P(m | m; s-k).$$

This completes the proof of (67).

It should be emphasized that the justification of using the product of probabilities in (68) rests upon the fact that in our process the past is independent of the future. In other words, once we know that the system starts, say, from " m ," its subsequent behavior is independent of the way in which " m " was reached in the first place.

We introduce now the generating functions

$$(69) \quad h(n | m; z) = \sum_{s=1}^{\infty} P(n | m; s)z^s$$

$$(70) \quad g(n | m; z) = \sum_{s=1}^{\infty} P'(n | m; s)z^s,$$

and note that (67) is equivalent to

$$h(n | m; z) = g(n | m; z) + h(m | m; z)g(n | m; z),$$

or

$$(71) \quad g(n | m; z) = \frac{h(n | m; z)}{1 + h(n | m; z)}.$$

In particular,

$$(72) \quad g(n | n; z) = \frac{h(n | n; z)}{1 + h(n | n; z)} = 1 - \frac{1}{1 + h(n | n; z)},$$

and we also note that

$$(73) \quad \frac{dg(n | n; z)}{dz} = \frac{\frac{dh(n | n; z)}{dz}}{(1 + h(n | n; z))^2}.$$

From the definition of $g(n | n; z)$, we obtain

$$(74) \quad \lim_{z \rightarrow 1} g(n | n; z) = \sum_{s=1}^{\infty} P'(n | n; s)$$

$$(75) \quad \tau \lim_{z \rightarrow 1} \frac{dg(n | n; z)}{dz} = \sum_{s=1}^{\infty} s \tau P'(n | n; s).$$

It is from these formulas that we shall derive (65) and (66). We have, using (62)

$$h(n | n; z) = \frac{(-1)^{R+n}}{2^{2R}} \sum_{j=-R}^R \sum_{s=1}^{\infty} \left(\frac{jz}{R}\right)^s C_{R+j}^{(-n)} C_{R+n}^{(j)},$$

and since

$$1 = \frac{(-1)^{R+n}}{2^{2R}} \sum_{j=-R}^R C_{R+j}^{(-n)} C_{R+n}^{(j)},$$

we obtain

$$(76) \quad 1 + h(n | n; z) = \frac{(-1)^{R+n}}{2^{2R}} \sum_{j=-R}^R \frac{1}{1 - \frac{j}{R} z} C_{R+j}^{(-n)} C_{R+n}^{(j)}.$$

All terms in the sum on the right hand side of (76) are regular at $z=1$ except the term corresponding to $j=R$, which has a simple pole at that point. Thus we can write

$$1 + h(n | n; z) = p(z) + \frac{(-1)^{R+n}}{2^{2R}} C_{2R}^{(-n)} C_{R+n}^{(R)} \frac{1}{1-z},$$

where $p(z)$ is regular at $z=1$. We see that

$$\lim_{z \rightarrow 1} (1 + h(n | n; z)) = \infty$$

and hence, using (72) and (74)

$$\sum_{s=1}^{\infty} P'(n | n; s) = 1.$$

It is easy to see that

$$\frac{(-1)^{R+n}}{2^{2R}} C_{2R}^{(-n)} C_{R+n}^{(R)} = \frac{1}{2^{2R}} \frac{(2R)!}{(R+n)!(R-n)!},$$

and, denoting this expression by ω , we have (for $|z| > 1$)

$$\frac{dg(n | n; z)}{dz} = \frac{(1-z)^2 p'(z) + \omega}{[(1-z)p(z) + \omega]^2},$$

and hence

$$\lim_{z \rightarrow 1} \frac{dg(n | n; z)}{dz} = \frac{1}{\omega}.$$

This together with (75) yields (66).

The above considerations can be extended to more general processes. However, Markoffian processes (*i.e.*, processes for which (68) is valid) are still the only ones for which one can also calculate the "fluctuation" of the recurrence time, namely, the quantity

$$(77) \quad \sum_{s=1}^{\infty} s^2 \tau^2 P'(n | n; s) - \theta_n^2.$$

Without going into the details, let us mention that (77) can be calculated in terms of

$$\lim_{z \rightarrow 1} \frac{d^2 g(n | n; z)}{dz^2}.$$

The fluctuation (77) gives us a measure of stability of the mean recurrence time inasmuch as it permits us to estimate how likely (or unlikely) it is to get a specified deviation of the actual recurrence time from the mean. It may seem that since the generating function $g(n | n; z)$ is known explicitly it should be easy to get an explicit expression for $P'(n | n; s)$. This, however, is not the case. We have not succeeded in finding such an expression, except for $P'(0 | 0; s)$, and even then we had to use a different method. We shall give a brief description of this method. Let

$$P(n | m; 1) = p_{nm}.$$

Then,

$$P'(n | n; s) = \sum'_{m_1, \dots, m_{s-1}} p_{nm_1} p_{m_1 m_2} \cdots p_{m_{s-1} n},$$

where the accent on the summation sign indicates that $m_j \neq n, j = 1, 2, \dots, s-1$. Now let

$$\epsilon_i = \begin{cases} 0 & \text{if } i = n \\ 1 & \text{if } i \neq n. \end{cases}$$

Noticing that

$$\epsilon_i^2 = \epsilon_i,$$

we can write

$$P'(n | n; s) = \sum_{m_1, \dots, m_{s-1}} p_{nm_1} \epsilon_{m_1} p_{m_1 m_2} \epsilon_{m_2} p_{m_2 m_3} \cdots \epsilon_{m_{s-2}} p_{m_{s-2} m_{s-1}} \epsilon_{m_{s-1}} p_{m_{s-1} n},$$

where the summation is now extended over all m_j . If B is the matrix

$$((p_{nm})),$$

and B_1 the matrix

$$((\epsilon_n p_{nm} \epsilon_m)),$$

we see that

$$(78) \quad P'(n | n; s) = (n, n) \text{ element of } BB_1^{s-2}B.$$

We may note that B_1 is obtained from B by crossing out the n th row and the n th column of the latter, and replacing them by a row and column consisting entirely of zeros. If B_1 can be explicitly diagonalized, that is, written in the form

$$B_1 = P_1 \begin{pmatrix} \mu_1 & & 0 \\ & \mu_2 & \\ 0 & & \ddots \end{pmatrix} Q_1,$$

where

$$P_1 Q_1 = I$$

one can calculate $P'(n | n; s)$, explicitly using (78).

We have applied this method to the Ehrenfest model, but only in the case when the middle (zeroth) row and column of B are replaced by a row and column consisting entirely of zeros have we been able to diagonalize explicitly the resulting matrix B_1 . The diagonalization proceeds very much as in Section 4, but it has proved necessary to distinguish between the cases when R is even or odd. In case R is even, we were able to derive the formula

$$(79) \quad P'(0 | 0; s) = -\frac{1}{2^{2R-1}} \frac{R+1}{2R} \sum \left(\frac{j}{R}\right)^{s-2} C_{R-j}^{(-1)} C_{R-1}^{(j)}, \quad s \geq 2,$$

where the summation is extended over all odd integers j between $-R$ and R . The details of the derivation are somewhat tedious and will not be reproduced here. Formula (79) furnishes a partial solution to a question left open by Wang and Uhlenbeck [1].

References

1. An extensive list of references to the physical literature can be found in the following articles: G. E. Uhlenbeck and L. S. Ornstein, On the theory of Brownian motion, *Phys. Rev.* 36 (1930) pp. 823–841, M. C. Wang and G. E. Uhlenbeck, On the theory of Brownian motion II, *Rev. Mod. Phys.* 17 (1945) pp. 323–342. For a very complete summary of earlier results see the important paper of Smoluchowski, *Drei Vorträge über Diffusion, Brownsche Molekularbewegung und Koagulation von Kolloidteilchen*, *Phys. Zeit.* 17 (1916) pp. 557–571 and 585–599.
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12. See the third article in [1] p. 568.

VIBRATION MODES OF TAPERED BEAMS

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The vibration modes of harmonically oscillating thin beams are obtained by solving the differential equation

$$(1) \quad (d^2/dx^2)(EI d^2y/dx^2) - \rho\omega^2 y = 0$$

subject to certain boundary conditions. In this differential equation, x is the distance along the beam, y is the amplitude of the transverse vibration, E is Young's modulus for the beam material, I is the cross-sectional moment of inertia of the beam, ρ is its linear density, and ω is the circular frequency of vibration.